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Project-Team RAPSODI

Reliable numerical approximations of dissipative systems

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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Project-Team RAPSODI

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2 Overall objectives

2.1 Overall objectives

Together with the diffusion of scientific computing, there has been a recent and impressive increase of the demand for numerical methods. The problems to be addressed are everyday more complex and require specific numerical algorithms. The quality of the results has to be accurately assessed, so that in-silico experiments results can be trusted. Nowadays, producing such reliable numerical results goes way beyond the abilities of isolated researchers, and must be carried out by structured teams.

The topics addressed by the RAPSODI project-team belong to the broad theme of numerical methods for the approximation of solutions of systems of partial differential equations (PDEs). Besides standard convergence properties, a good numerical method for approximating a physical problem has to satisfy at least the following three criteria:

(a) preservation at the discrete level of some crucial features of the solution, such as positivity of solutions, conservation of prescribed quantities (e.g. mass, the decay of physically motivated entropies etc.);

(b) provide accurate numerical approximations at a reasonable computational cost (and ultimately maximize the accuracy at a fixed computational effort);

(c) robustness with respect to physical conditions: the computational cost for a given accuracy should be essentially insensitive to change of physical parameters.

We aim to develop methods fulfilling the above quality criteria for physical models which all display a dissipative behavior, and that are motivated by industrial collaborations or multidisciplinary projects. In particular, we have identified a couple of specific situations we plan to investigate: models from corrosion science (in the framework of nuclear waste repository) [71], low-frequency electromagnetism [88], and mechanics of complex inhomogeneous fluids arising in avalanches [80] or in porous media [72].

Ideally, we should allow ourselves to design entirely new numerical methods. For some applications however (often in the context of industrial collaborations), the members of the team have to compose with existing codes. The numerical algorithms have thus to be optimized under this constraint.

2.2 Scientific context

Some technological bottlenecks related to points (a)–(c) mentioned above are well identified. In particular, it appears that a good numerical method should handle general meshes, so that dynamic mesh adaptation strategies can be used in order to achieve (b). But it should also be of the highest possible order while remaining stable in the sense of (a), and robust in the sense of (c). There have been numerous research contributions on each point of (a)–(c) in the last decades, in particular for solving each difficulty separately, but combining them still leads to unsolved problems of crucial interest.

Let us mention for example the review paper by J. Droniou [97], where it is highlighted that all the linear methods for solving diffusion equations on general meshes suffer from the same lack of monotonicity and preserve neither the positivity of the solutions nor the decay of the entropy. Moreover, there is no complete convergence proof for the nonlinear methods exposed in [97]. The first convergence proof for a positivity preserving and entropy diminishing method designed to approximate transient dissipative equations on general meshes was proposed very recently in [83]. The idea and the techniques introduced in [83] should be extended to practical applications.

In systems of PDEs, the values of the physical parameters often change the qualitative behavior of the solutions. Then, one challenge in the numerical approximation of such systems is the design of methods which can be applied for a large range of parameters, as in particular in the regime of singular perturbations. Such schemes, called *asymptotic-preserving* (AP) schemes [104], are powerful tools as they

allow the use of the same scheme for a given problem and for its limit with fixed discretization parameters. In many cases, the AP property of numerical schemes is just empirically established, without any rigorous proof. We aim to extend the techniques recently introduced in [77] for the drift-diffusion system, and based on the control of the numerical dissipation of entropy, to other dissipative systems in order to prove the AP property of numerical schemes.

The question of the robustness of the numerical methods with respect to the physical parameters is also fundamental for fluid mixture models. The team already developed such schemes for the variable density Navier–Stokes system [79, 80]. We aim to propose new ones for more complex models with the same philosophy in mind. On the one hand, we will be interested in high-order schemes, which must be as simple as possible in view of 3D practical implementations. Let us stress that combining high order accuracy and stability is very challenging. On the other hand, the optimization of the computation will have to be considered, in particular with the development of some a posteriori error estimators. Impressive progresses have been achieved in this field [93], allowing important computational savings without compromising the accuracy of the results. Recently, we successfully applied this strategy to the Reissner–Mindlin model arising in solid mechanics [90], the dead-oil model for porous media flows [82], or the Maxwell equations in their quasi-static approximation for some eddy current problems [88, 89]. We aim to develop new a posteriori estimators for other dissipative systems, like fluid mixture models.

In a nutshell, our goal is to take advantage of and extend the most recent breakthroughs of the mathematical community to tackle in an efficient way some application-guided problems coming either from academics or from industrial partners. To this end, we shall focus on the following objectives, which are necessary for the applications we have in mind:

1. Design and analysis of structure-preserving numerical methods.
2. Computational optimization.

3 Research program

3.1 Design and analysis of structure-preserving schemes

3.1.1 Numerical analysis of nonlinear numerical methods

Up to now, almost all numerical methods dedicated to degenerate parabolic problems that the mathematicians are able to analyze rely on the use of mathematical transformations (like e.g. the Kirchhoff's transform). It forbids the extension of the analysis to complex realistic models. The methods used in the industrial codes for solving such complex problems rely on the use of what we call NNM, i.e. on methods that preserve all the nonlinearities of the problem without reducing them thanks to artificial mathematical transforms. Our aim is to take advantage of the recent breakthrough proposed by C. Cancès and C. Guichard [4] and [83] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness with respect to physical parameters etc.).

3.1.2 Design and analysis of asymptotic-preserving schemes

There has been an extensive effort in the recent years to develop numerical methods for diffusion equations that are robust with respect to heterogeneities, anisotropy, and the mesh (see for instance [97] for an extensive discussion on such methods). On the other hand, the understanding of the role of nonlinear stability properties in the asymptotic behaviors of dissipative systems increased significantly in the last decades (see for instance [84, 106]).

Recently, C. Chainais-Hillairet and co-authors [77, 85, 86] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization characteristic parameters, or in the long-time asymptotic. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes etc.) are required in [77, 85, 86]. The schemes proposed in [4] and [83] allow to handle nonlinear test functions in the analysis without restrictions on the mesh and on the anisotropy of the

problem. Combining the nonlinear schemes *à la* [83] with the methodology of [77, 85, 86] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would also be robust under adaptive mesh refinement.

3.1.3 Design and stability analysis of numerical methods for low-Mach models

We aim at extending the range of the `NS2DDV-M` software (cf. [62]) by introducing new physical models, like for instance the low-Mach model, which gives intermediate solutions between the compressible Navier–Stokes model and the incompressible Navier–Stokes one. This model was introduced in [105] as a limiting system which describes combustion processes at low Mach number in a confined region. Within this scope, we will propose a theoretical study for proving the existence of weak solutions for a particular class of models for which the dynamic viscosity of the fluid is a specific function of the density. We will also propose the extension of a combined Finite Volume-Finite Element method, initially developed for the simulation of incompressible and variable density flows, to this class of models.

3.2 Optimizing the computational efficiency

3.2.1 High-order nonlinear numerical methods

The numerical experiments carried out in [83] show that in case of very strong anisotropy, the convergence of the proposed NNM becomes too slow (less than first order). Indeed, the method appears to strongly overestimate the dissipation. In order to make the method more competitive, it is necessary to estimate the dissipation in a more accurate way. Preliminary numerical results show that second-order accuracy in space can be achieved in this way. One also aims to obtain (at least) second-order accuracy in time without jeopardizing the stability. For many problems, this can be done by using so-called two-step backward differentiation formulas (BDF2) [100].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider Residual Distribution schemes, that appear as an alternative to Finite Volume methods. Residual Distribution schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D entails reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [103, 107], with high-order accuracy [65, 66], or for parabolic problems [63, 64] make them very competitive. Relying on these breakthroughs, we aim at designing new Residual Distribution schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2 *A posteriori* error control

The question of the a posteriori error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuška and Rheinboldt more than thirty years ago [69], a posteriori error estimators have been widely studied. We will take advantage of the huge corresponding bibliographical database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g. [88, 89]) to the temporal magnetodynamic one, for which space-time a posteriori error estimators have to be developed. A space-time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop a posteriori estimators for the variable density Navier–Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [79, 80] we developed combines features from Finite Elements and Finite Volumes. Fortunately, there exists a significant literature on the subject. Some recent references are devoted to the unsteady Navier–Stokes model in the Finite Element context [75, 101]. In the Finite Volume context, recent references deal with unsteady convection-diffusion equations [68, 82, 96, 109]. We want to adapt some of these results to the variable density Navier–Stokes system, and to be able to design an efficient space-time remeshing algorithm.

3.2.3 Efficient computation of pairwise interactions in large systems of particles

Many systems are modeled as a large number (N) of pointwise individuals with pairwise interaction, i.e. with $N(N-1)/2$ interactions. Such systems are ubiquitous, they are found in chemistry (Van der Waals interaction between atoms), in astrophysics (gravitational interactions between stars, galaxies or galaxy clusters), in biology (flocking behavior of birds, schooling of fish) or in the description of crowd motions. Building on the special structure of convolution type of the interactions, the team develops computation methods based on the nonuniform Fast Fourier Transform [102]. This reduces the $O(N^2)$ naive computational cost of the interactions to $O(N \log N)$, allowing numerical simulations involving millions of individuals.

4 Application domains

4.1 Porous media flows

Porous media flows are of great interest in many contexts, like, e.g. oil engineering, water resources management, nuclear waste repository management, or carbon dioxide sequestration. We refer to [72, 73] for an extensive discussion on porous media flow models.

From a mathematical point of view, the transport of complex fluids in porous media often leads to possibly degenerate parabolic conservation laws. The porous rocks can be highly heterogeneous and anisotropic. Moreover, the grids on which one intends to solve numerically the problems are prescribed by the geological data, and might be nonconformal with cells of various shapes. Therefore, the schemes used for simulating such complex flows must be particularly robust.

4.2 Corrosion and concrete carbonation

The team is interested in the theoretical and numerical analysis of mathematical models describing the degradation of materials, as concrete carbonation and corrosion. The study of such models is an important environmental and industrial issue. Atmospheric carbonation degrades reinforced concretes and limits the lifetime of civil engineering structures. Corrosion phenomena issues occur for instance in the reliability of nuclear power plants and the nuclear waste repository. The study of the long time evolution of these phenomena is of course fundamental in order to predict the lifetime of the structures.

From a mathematical point of view, the modeling of concrete carbonation (see [67]) as the modeling of corrosion in an underground repository (DPCM model developed by Bataillon et al. [71]) lead to systems of PDEs posed on moving domains. The coupling between convection-diffusion-reaction equations and moving boundary equations leads to challenging mathematical questions.

4.3 Complex fluid flows

The team is interested in numerical methods for the simulation of systems of PDEs describing complex flows, like for instance mixture flows, granular gases, rarefied gases, or quantum fluids.

Variable-density, low-Mach flows have been widely studied in the recent literature because of their applicability in various phenomena such as flows in high-temperature gas reactors, meteorological flows, flows with convective and/or conductive heat transfer or combustion processes. In such cases, the resolution of the full compressible Navier–Stokes system is not adapted, because of the sound waves' speed. The Boussinesq incompressible model is not a better alternative for such low-speed phenomena, because the compressibility effects cannot be totally cancelled due to large variations of temperature and density. Consequently, some models have been formally derived, leading to the filtering of the acoustic waves by the use of some formal asymptotic expansions and two families of methods have been developed in the literature in order to compute these flows. We are interested in particular in the so-called pressure-based methods, which are more robust than density-based solvers, although their range of validity is in general more limited.

The kinetic theory of molecular gases models a gas as a system of elastically colliding spheres, conserving mechanical energy during impact. Once initialized, it takes to a molecular gas no more than a few collisions per particle to relax to its equilibrium state, characterized by a Maxwellian velocity distribution

and a certain homogeneous density (in the absence of external forces). A granular gas is a system of dissipatively colliding, macroscopic particles (grains). This slight change in the microscopic dynamics (converting energy into heat) causes drastic changes in the behavior of the gas: granular gases are open systems, which exhibit self-organized spatio-temporal cluster formations, and have no equilibrium distribution. They can be used to model silos, avalanches, pollen or planetary rings.

Quantum models can be used to describe superfluids, quantum semiconductors, weakly interacting Bose gases, or quantum trajectories of Bohmian mechanics. They have attracted considerable attention in the last decades, due in particular to the development of nanotechnology applications. To describe quantum phenomena, there exists a large variety of models. In particular, there exist three different levels of description: microscopic, mesoscopic, and macroscopic. The quantum Navier–Stokes equations deal with a macroscopic description in which the quantum effects are taken into account through a third-order term called the quantum Bohm potential. This Bohm potential arises from the fluid dynamical formulation of the single-state Schrödinger equation. The nonlocality of quantum mechanics is approximated by the fact that the equations of state do not only depend on the particle density but also on its gradient. These equations were employed to model field emissions from metals and steady-state tunneling in metal-insulator-metal structures, and to simulate ultra-small semiconductor devices.

4.4 Stratigraphy

The knowledge of the geology is a prerequisite before simulating flows within the subsoil. Numerical simulations of the geological history thanks to stratigraphy numerical codes allow to complete the knowledge of the geology where experimental data are lacking. Stratigraphic models consist in a description of the erosion and sedimentation phenomena at geological scales.

The characteristic time scales for the sediments are much larger than the characteristic time scales for the water in the river. However, the (time-averaged) water flux plays a crucial role in the evolution of the stratigraphy. Therefore, defining appropriate models that take the coupling between the rivers and the sediments into account is fundamental and challenging. Once the models are at hand, efficient numerical methods must be developed.

4.5 Low-frequency electromagnetism

Numerical simulation is nowadays an essential tool in order to design electromagnetic systems, by estimating the electromagnetic fields generated in a wide variety of devices. An important challenge for many applications is to quantify the intensity of the electric field induced in a conductor by a current generated in its neighborhood. In the low-frequency regime, we can for example cite the study of the impact on the human body of a high-tension line or, for higher frequencies, the one of a smartphone. But the ability to simulate accurately some electromagnetic fields is also very useful for nondestructive control, in the context of the maintenance of nuclear power stations for example. The development of efficient numerical tools, among which a posteriori error estimators, is consequently necessary to reach a high precision of calculation in order to provide as reliable estimations as possible.

5 New software and platforms

5.1 Platform `ParaSkel++`

`ParaSkel++` is a parallel C++ platform for the optimized, arbitrary-order, 2/3D numerical approximation of PDEs on general meshes using skeletal Galerkin methods.

Skeletal Galerkin methods form a vast class of numerical methods for the approximation of PDEs that is based on the following 2 building principles:

- the degrees of freedom (DOF) of the method split into (i) skeletal DOF, attached to the geometrical entities composing the mesh skeleton (vertices, edges, faces) and common, locally, to all cells sharing the geometrical entity in question, which prescribe the conformity properties of the underlying functional space, and (ii) bulk DOF, attached to the interior of the cell, that are not shared between

adjacent elements and which play no role in the prescription of the conformity properties of the functional space;

- the global discrete bilinear form writes as the sum of strictly local (to each cell) contributions.

The very structure of skeletal methods grants them the property of being amenable to static condensation, i.e. bulk DOF can be locally eliminated in terms of the skeletal DOF of the cell in question. The final global system to solve thus writes in terms of the skeletal DOF only, whence the vocable of "skeletal" method. Due to the local character of the computations to perform to assemble the system, skeletal methods are highly parallelizable. The class of skeletal methods encompasses in particular (conforming and nonconforming) FE methods, and virtual-like Galerkin methods (VEM, HDG, HHO...). It does not contain DG methods.

The `ParaSkel++` platform offers an optimized and unified C++ architecture for the implementation of arbitrary-order skeletal Galerkin methods on general 2/3D meshes. The development of this platform has begun in February 2020, and is expected to last (at least) 30 months. The P.I. of the project is S. Lemaire, and the main developer is L. Beaude.

5.2 Other codes

The code `FPmuRNA`, that has been used to produce the numerical simulations of the article "A Fokker–Planck approach to the study of robustness in gene expression" [30], has been published online as open-source (available at gitlab.inria.fr/herda/fpmurna). `FPmuRNA` is a Matlab code developed by M. Herda.

The code `KinDiff`, that has been used to produce the numerical simulations of the article "Hypocoercivity and diffusion limit of a Finite Volume scheme for linear kinetic equations" [15], has been published online as open-source (available at gitlab.com/thoma.rey/FV_HipoDiff). `KinDiff`, developed by M. Bessemoulin-Chatard (CNRS and Université de Nantes), M. Herda, and T. Rey, consists in a Python code and a Jupyter Notebook. It approximates the solutions to the kinetic Fokker–Planck and linear BGK equations in a unidimensional periodic domain in space and a symmetric bounded unidimensional domain in velocity. Its outputs are the discretization of the distribution function in the phase space as well as the moments, along with some visualizations of these quantities. Kinetic equations display asymptotic behaviors such as return to equilibrium in large time, or convergence towards macroscopic equations in the diffusive limit. The Finite Volume method implemented within `KinDiff` reproduces these asymptotics at the discrete level.

The code [99], that has been used to produce the numerical simulations of the article "Finite Volumes for the Stefan–Maxwell cross-diffusion system" [50], has been published online as open-source (available at 10.5281/zenodo.3934285). This Julia code, developed by C. Cancès, V. Ehrlacher, and L. Monasse, simulates the Stefan–Maxwell equations on Cartesian grids thanks to an entropy-diminishing Two-Point Flux Approximation Finite Volume scheme.

The code that has been used to perform the computer-assisted proofs of the article "Existence of traveling wave solutions for the Diffusion Poisson Coupled Model: a computer-assisted proof" [48] has been published online as open-source (available at sites.google.com/site/maximebreden/research). This Matlab code has been developed by M. Breden, C. Chainais-Hillairet, and A. Zurek.

6 New results

6.1 Modeling and numerical simulation of complex fluids

In [45], C. Cancès et al. establish an error estimate, within the generic framework for the spatial discretisation of partial differential equations of the Gradient Discretisation Method (GDM), for a class of degenerate parabolic problems. This result is obtained under very mild regularity assumptions on the exact solution. Their study covers well-known models like the porous medium equation and the fast diffusion equations, as well as the strongly degenerate Stefan problem. Several schemes are then compared in a last section devoted to numerical results.

In [40], C. Cancès et al. propose a P^1 Finite Element scheme with mass-lumping for a model of two incompressible and immiscible phases in a porous media flow. They prove the dissipation of the free

energy and the existence of a solution to the nonlinear scheme. They also present numerical simulations to illustrate the behavior of the scheme.

In [51], C. Cancès et al. prove the existence of weak solutions to a system of two diffusion equations that are coupled by a pointwise volume constraint. The time evolution is given by gradient dynamics for a free energy functional. Their primary example is a model for the demixing of polymers, the corresponding energy is the one of Flory, Huggins and deGennes. Due to the nonlocality in the equations, the dynamics considered here is qualitatively different from the one found in the formally related Cahn–Hilliard equations. Their angle of attack stems from the theory of optimal mass transport, that is, they consider the evolution equations for the two components as two gradient flows in the Wasserstein distance with one joint energy functional that has the volume constraint built in. The main difference with their previous work [81] is the nonlinearity of the energy density in the gradient part, which becomes singular at the interface between pure and mixed phases.

In [23], C. Cancès, N. Peton et al. propose a new water flow-driven forward stratigraphic model. Stratigraphy is a discipline of physics that aims at predicting the geological composition of the subsoil. The model enjoys the following particularities. First, the water surface flow is modelled at the continuous level, in opposition to what is currently done in this community. Second, the model incorporates a constraint on the erosion rate. A stable numerical scheme is proposed to simulate the model.

In [17], C. Calgaro, C. Colin, and E. Creusé propose a combined Finite Volume-Finite Element scheme for the solution of a specific low-Mach model expressed in the velocity, pressure and temperature variables. The dynamic viscosity of the fluid is given by an explicit function of the temperature, leading to the presence of a so-called Joule term in the mass conservation equation. First, they prove a discrete maximum principle for the temperature. Second, the numerical fluxes defined for the Finite Volume computation of the temperature are efficiently derived from the discrete Finite Element velocity field obtained by the solution of the momentum equation. Several numerical tests are presented to illustrate the theoretical results and to underline the efficiency of the scheme in terms of convergence rates.

In [37], C. Calgaro and E. Creusé introduce a Finite Volume method to approximate the solution of a convection-diffusion equation involving a Joule term. They propose a way to discretize this so-called "Joule effect" term in a consistent manner with respect to the nonlinear diffusion one, in order to ensure some maximum principle properties on the solution. They investigate the numerical behavior of the scheme on two original benchmarks.

In [53], T. Rey et al. review recent mathematical results in kinetic granular materials, especially for those which arose since the last review by Villani on the same subject. This model describes the nonequilibrium behavior of materials composed of a large number of interacting, nonnecessarily microscopic particles, such as grains or planetary rings. This theoretical knowledge is then used to validate a new high-order numerical method for this equation, highlighting through numerics some theoretical open problems.

In [30], M. Herda et al. study several Fokker–Planck equations arising from a stochastic chemical kinetic system modeling a gene regulatory network in biology. The densities solving the Fokker–Planck equations describe the joint distribution of the messenger RNA and micro RNA content in a cell. They provide theoretical and numerical evidences that the robustness of the gene expression is increased in the presence of micro RNA. At the mathematical level, increased robustness shows in a smaller coefficient of variation of the marginal density of the messenger RNA in the presence of micro RNA. These results follow from explicit formulas for solutions. Moreover, thanks to dimensional analyses and numerical simulations they provide qualitative insight into the role of each parameter in the model. As the increase of gene expression level comes from the underlying stochasticity in the models, they eventually discuss the choice of noise in their models and its influence on their results.

In [48], C. Chainais-Hillairet, A. Zurek et al. present and apply a computer-assisted method in order to prove the existence of traveling wave solutions to the Diffusion Poisson Coupled Model arising in corrosion modeling. They also establish a precise and certified description of the solutions.

6.2 Numerical simulation in low-frequency electromagnetism

In [29], E. Creusé et al. study the $\mathbf{A}-\varphi-\mathbf{B}$ magnetodynamic Maxwell system, given in its potential and space-time formulation. First, the existence of strong solutions with the help of the theory of Showalter on

degenerate parabolic problems is established. Second, using energy estimates, existence and uniqueness of the weak solution to the $\mathbf{A}-\varphi-\mathbf{B}$ system is deduced.

In [43], F. Chave, S. Lemaire et al. introduce a three-dimensional Hybrid High-Order (HHO) method for the magnetostatics problem. The proposed method is easy to implement, supports general polyhedral meshes, and allows for arbitrary orders of approximation.

In [54], F. Chave, S. Lemaire et al. prove a discrete version of the first Weber inequality on three-dimensional hybrid spaces spanned by vectors of polynomials attached to the elements and faces of a polyhedral mesh. They then study two HHO methods for the approximation of the magnetostatics model, in both its (first-order) field and (second-order) vector potential formulations. These methods are applicable on general polyhedral meshes with star-shaped elements, and allow for arbitrary orders of approximation. Leveraging the previously established discrete Weber inequality, they perform a comprehensive analysis of the two methods, that they finally validate on a set of test-cases.

6.3 Structure-preserving numerical methods

In [41], C. Chainais-Hillairet and M. Herda apply an iterative energy method *à la* de Giorgi in order to establish L^∞ bounds for numerical solutions of noncoercive convection-diffusion equations with mixed Dirichlet-Neumann boundary conditions.

In [36], C. Chainais-Hillairet et al. propose some Finite Volume schemes for unipolar energy-transport models. Using a reformulation in dual entropy variables, they show the decay of a discrete entropy with control of the discrete entropy dissipation.

In [47], C. Chainais-Hillairet et al. develop their work [36]. They establish a priori estimates which lead to the existence of a solution to the scheme, and they prove the exponential decay of the discrete relative entropy towards the thermal equilibrium. Moreover, numerical results assess the good behavior of the numerical schemes.

In [19], C. Cancès, C. Chainais-Hillairet, B. Gaudeul et al. consider an unipolar degenerate drift-diffusion system arising in the modeling of organic semiconductors. They design four different Finite Volume schemes based on four different formulations of the fluxes. They provide a stability analysis and existence results for the four schemes; the convergence is established for two of them.

In [38], C. Cancès, C. Chainais-Hillairet, B. Gaudeul et al. consider an unipolar degenerate drift-diffusion system where the relation between the concentration of the charged species c and the chemical potential h is $h(c)=\log\frac{c}{1-c}$. For four different Finite Volume schemes based on four different formulations of the fluxes of the problem, they discuss stability and existence results. For two of them, they report a convergence proof. Numerical experiments illustrate the behavior of the different schemes.

In [26], C. Cancès et al. propose a Finite Element scheme for the numerical approximation of degenerate parabolic problems in the form of a nonlinear anisotropic Fokker–Planck equation. The scheme is energy-stable, only involves physically motivated quantities in its definition, and is able to handle general unstructured grids. Its convergence is rigorously proven thanks to compactness arguments, under very general assumptions. Although the scheme is based on Lagrange Finite Elements of degree 1, it is locally conservative after a local post-processing giving rise to an equilibrated flux. This also allows to derive a guaranteed a posteriori error estimate for the approximate solution. Numerical experiments are presented in order to give evidence of a very good behavior of the proposed scheme in various situations involving strong anisotropy and drift terms.

In [25], C. Cancès et al. study a time-implicit Finite Volume scheme for the degenerate Cahn–Hilliard model proposed in [98] and studied mathematically in [81]. The scheme is shown to preserve the key properties of the continuous model, namely mass conservation, positivity of the concentrations, the decay of the energy, and the control of the entropy dissipation rate. This allows to establish the existence of a solution to the nonlinear algebraic system corresponding to the scheme. Furthermore, C. Cancès et al. show thanks to compactness arguments that the approximate solution converges towards a weak solution to the continuous problem as the discretization parameters tend to 0. Numerical results illustrate the behavior of the numerical scheme.

In [39], C. Cancès and B. Gaudeul propose a Two-Point Flux Approximation Finite Volume scheme for the approximation of the solutions to an entropy dissipative cross-diffusion system. The scheme is shown to preserve several key properties of the continuous system, among which positivity and decay of the entropy. Numerical experiments illustrate the behavior of the scheme.

In [22], C. Cancès and B. Gaudeul study a Two-Point Flux Approximation Finite Volume scheme for a cross-diffusion system. The scheme is shown to preserve the key properties of the continuous system, among which the decay of the entropy. The convergence of the scheme is established thanks to compactness properties based on the discrete entropy-entropy dissipation estimate. Numerical results illustrate the behavior of the scheme.

In [50], C. Cancès et al. propose a provably convergent Finite Volume scheme for the so-called Stefan–Maxwell model, which describes the evolution of the composition of a multi-component mixture and reads as a cross-diffusion system. The proposed scheme relies on a Two-Point Flux Approximation, and preserves at the discrete level some fundamental theoretical properties of the continuous model, namely the non-negativity of the solutions, the conservation of mass, and the preservation of the volume-filling constraints. In addition, the scheme satisfies a discrete entropy-entropy dissipation relation, very close to the relation which holds at the continuous level. In this article, C. Cancès et al. present the scheme together with its numerical analysis, and finally illustrate its behavior with some numerical results.

In [21], C. Cancès et al. propose a variational Finite Volume scheme for the computation of Wasserstein gradient flows. The discrete solution is the minimizer of a discrete action, keeping track at the discrete level of the optimal character of the gradient flow. The spatial discretization relies on upstream mobility fluxes, while an implicit linearization of the Wasserstein distance is used in order to reduce the computational cost by avoiding an inner time-stepping as in the related contributions of the literature.

In [13], R. Bailo et al. study an implicit Finite Volume scheme for nonlinear, nonlocal aggregation-diffusion equations which exhibit a gradient flow structure, recently introduced in [70]. Crucially, this scheme keeps the dissipation property of an associated fully discrete energy, and does so unconditionally with respect to the time step. The main contribution in this work is to show the convergence of the method under suitable assumptions on the diffusion functions and potentials involved.

In [57], A. Natale et al. construct and analyze Two-Point Flux Approximation Finite Volume discretizations of the quadratic optimal transport problem in its dynamic form. They show numerically that these types of discretizations are prone to form instabilities in their more natural implementation, and propose a variation based on nested meshes in order to overcome these issues. Moreover, they introduce a strategy based on the barrier method to solve the discrete optimization problem.

In [58], T. Rey et al. focus on the stability properties of some recently introduced spectral methods that preserve equilibrium. Thanks to the high accuracy and the possibility to use fast algorithms, such methods represent an effective way to approximate the Boltzmann collision operator. On the other hand, the loss of some local invariants usually leads to the wrong long-time behavior. In this paper, using the perturbation argument developed by Filbet and Mouhot for the homogeneous Boltzmann equation, the authors prove stability, convergence, and spectrally accurate long-time behavior of the equilibrium-preserving approach.

In [44], T. Rey et al. present a new Finite Volume method for computing numerical approximations of a system of nonlocal transport equations modeling interacting species. In this work, the nonlocal continuity equations are treated as conservative transport equations with a nonlocal, nonlinear, rough velocity field. Some properties of the method are analyzed, and numerical simulations are performed.

In [14], I. Lacroix-Violet et al. focus on the numerical integration in time of nonlinear Schrödinger equations using different methods preserving the energy or a discrete analog of it. In particular, they give a rigorous proof of the order of the relaxation method (presented in [76] for cubic nonlinearities) and they propose a generalized version that allows to deal with general power law nonlinearities. Numerical simulations for different physical models show the efficiency of these methods.

6.4 Cost reduction for numerical methods

In [34], S. Lemaire presents a unifying viewpoint on Hybrid High-Order [94] and Virtual Element [74] methods on general polytopal meshes in dimension 2 or 3, in terms of both formulation and analysis. The focus is on a model Poisson problem. To bridge the two paradigms, (i) he transcribes the (conforming) Virtual Element method into the Hybrid High-Order framework and (ii) proves H^m approximation properties for the local polynomial projector in terms of which the local Virtual Element discrete bilinear form is defined. This allows him to perform a unified analysis of Virtual Element/Hybrid High-Order methods, that differs from standard Virtual Element analyses by the fact that the approximation properties of the underlying virtual space are not explicitly used. As a complement to this unified analysis, he also

studies interpolation in local virtual spaces, shedding light on the differences between the conforming and nonconforming cases.

In [55], I. Lacroix-Violet et al. introduce a new class of numerical methods for the time integration of evolution equations set as Cauchy problems of ODEs or PDEs. The systematic design of these methods mixes the Runge–Kutta collocation formalism with collocation techniques, in such a way that the methods are linearly implicit and have high order. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods are expected to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so.

In [35], S. Bassetto, C. Cancès et al. propose an efficient nonlinear solver for the resolution of the Richards equation. It is based on variable switching and can be easily implemented thanks to a fictitious variable allowing to describe both the saturation and the pressure. Numerical experiments show that the method enables to use Newton's method with large time steps, a reasonable number of iterations, and in regions where the pressure-saturation relationship is given by a graph.

In [24], C. Cancès and D. Maltese propose a reduced model for the migration of hydrocarbons in heterogeneous porous media. Their model keeps track of the time variable. This allows to compute steady-states that cannot be reached by the commonly used ray-tracing and invasion-percolation algorithms. An efficient Finite Volume scheme allowing for very large time steps is then proposed.

6.5 Asymptotic analysis

In [27], C. Chainais-Hillairet and M. Herda study the large-time behavior of the solutions to Finite Volume discretizations of convection-diffusion equations or systems endowed with non-homogeneous Dirichlet and Neumann type boundary conditions. Their results concern various linear and nonlinear models such as Fokker–Planck equations, porous media equations, or drift-diffusion systems for semiconductors. For all of these models, some relative entropy principle is satisfied and implies exponential decay to the stationary state. They show that in the framework of Finite Volume schemes on orthogonal meshes, a large class of two-point monotone fluxes preserves this exponential decay of the discrete solution to the discrete steady-state of the scheme.

In [20], C. Cancès, C. Chainais-Hillairet, M. Herda et al. analyze the large-time behavior of a family of nonlinear Finite Volume schemes for anisotropic convection-diffusion equations set in a bounded bidimensional domain and endowed with either Dirichlet and/or no-flux boundary conditions. They show that the solutions to the Two-Point Flux Approximation (TPFA) and Discrete Duality Finite Volume (DDFV) schemes under consideration converge exponentially fast towards their steady-state. The analysis relies on discrete entropy estimates and discrete functional inequalities. As a by-product of their analysis, they establish new discrete Poincaré–Wirtinger, Beckner and logarithmic Sobolev inequalities. Their theoretical results are illustrated by numerical simulations.

In [42], C. Chainais-Hillairet et al. introduce a nonlinear DDFV scheme for an anisotropic linear convection-diffusion equation with mixed boundary conditions and establish the exponential decay of the scheme towards its steady-state.

In [15], M. Herda, T. Rey et al. are interested in the asymptotic analysis of a Finite Volume scheme for one-dimensional linear kinetic equations, with either Fokker–Planck or linearized BGK collision operator. Thanks to appropriate uniform estimates, they establish that the proposed scheme is asymptotic-preserving in the diffusive limit. Moreover, they adapt to the discrete framework the hypocoercivity method proposed in [95] to prove the exponential return to equilibrium of the approximate solution. They obtain decay estimates that are uniform in the diffusive limit. Finally, they present an efficient implementation of the proposed numerical schemes, and perform numerous numerical simulations assessing their accuracy and efficiency in capturing the correct asymptotic behaviors of the models.

In [12], M. Herda et al. are interested in the large-time behavior of linear kinetic equations with heavy-tailed local equilibria. Their main contribution concerns the kinetic Lévy–Fokker–Planck equation, for which they adapt hypocoercivity techniques in order to show that solutions converge exponentially fast to the global equilibrium. Compared to the classical kinetic Fokker–Planck equation, the issues here concern the lack of symmetry of the nonlocal Lévy–Fokker–Planck operator and the understanding of its regularization properties. As a complementary related result, they also treat the case of the heavy-tailed BGK equation.

In [49], I. Lacroix-Violet et al. consider global weak solutions to compressible Navier–Stokes–Korteweg equations with density dependent viscosities, in a periodic domain $\Omega = \mathbb{T}^3$, with a linear drag term with respect to the velocity. The main result concerns the exponential decay to equilibrium of such solutions using log-Sobolev type inequalities. In order to show such a result, the starting point is a global weak-entropy solutions definition, introduced in [78]. Assuming extra assumptions on the shear viscosity when the density is close to vacuum and when the density tends to infinity, I. Lacroix-Violet et al. conclude the exponential decay to equilibrium. The result also covers the quantum Navier–Stokes system with a drag term.

In [16], T. Rey et al. propose a new mathematical model intended to describe dynamically the evolution of knowledge in structured societies of interacting individuals. This process, termed cumulative culture, has been extensively studied by evolutionary anthropologists, both theoretically and experimentally. Some of the mathematical properties of the new model are analyzed, and exponential convergence towards a global equilibrium is shown for a simplified model. A numerical method is finally proposed to simulate the complete model.

In [11], following the ideas of V. V. Zhikov and A. L. Pyatnitskii, and more precisely the stochastic two-scale convergence, B. Merlet et al. establish a homogenization theorem in a stochastic setting for two nonlinear equations: the equation of harmonic maps into the sphere, and the Landau–Lifshitz equation. Homogenization results for nonlinear problems are known to be difficult. In this particular case, the equations have strong nonlinear features; in particular, in general, their solutions are not unique. Here, the authors take advantage of the different equivalent definitions of weak solutions to the nonlinear problem to apply typical linear homogenization recipes.

6.6 Applied calculus of variations

In [33], B. Merlet et al. study a variational problem which models the behavior of topological singularities on the surface of a biological membrane in P_β-phase (see [108]). The problem combines features of the Ginzburg–Landau model in 2D and of the Mumford–Shah functional. As in the classical Ginzburg–Landau theory, a prescribed number of point vortices appears in the moderate energy regime; the model allows for discontinuities, and the energy penalizes their length. The novel phenomenon here is that the vortices have a fractional degree $1/m$ with m prescribed. Those vortices must be connected by line discontinuities to form clusters of total integer degrees. The vortices and line discontinuities are therefore coupled through a topological constraint. As in the Ginzburg–Landau model, the energy is parameterized by a small length scale $\varepsilon > 0$. B. Merlet et al. perform a complete Γ-convergence analysis of the model as $\varepsilon \downarrow 0$ in the moderate energy regime. Then, they study the structure of minimizers of the limit problem. In particular, the line discontinuities of a minimizer solve a variant of the Steiner problem.

In [28], B. Merlet et al. establish new results on the approximation of k-dimensional surfaces (k-rectifiable currents) by polyhedral surfaces with convergence in h-mass and with preservation of the boundary (the approximating polyhedral surface has the same boundary as the limit). This approximation result is required in the convergence study of [87].

In [32], B. Merlet et al. study a family of functionals penalizing oblique oscillations. These functionals naturally appear in some variational problems related to pattern formation and are somewhat reminiscent of those introduced by Bourgain, Brezis and Mironescu to characterize Sobolev functions. More precisely, for a function u defined on a tensor product $\Omega_1 \times \Omega_2$, the family of functionals $\{E_\varepsilon(u)\}_{\varepsilon>0}$ that they consider vanishes if u is of the form $u(x_1)$ or $u(x_2)$. They prove the converse property and related quantitative results. In particular, they describe the fine properties of functions with $\sup_\varepsilon E_\varepsilon(u) < \infty$ by showing that, roughly, such u is piecewise of the form $u(x_1)$ or $u(x_2)$ on domains separated by lines where the energy concentrates. It turns out that this problem naturally leads to the study of various differential inclusions, and has connections with branched transportation models.

In [59], M. Pegon studies large volume minimizers of isoperimetric problems derived from Gamow's liquid drop model for the atomic nucleus, involving the competition of a perimeter term and repulsive nonlocal potentials. Considering a large class of potentials, given by general radial nonnegative kernels which are integrable on $\mathbb{R}^n$, such as Bessel potentials, M. Pegon proves the existence of minimizers of arbitrarily large mass, provided that the first moment of the kernels is below an explicit threshold. This contrasts with the case of Riesz potentials, where minimizers do not exist above a critical mass. In addition, renormalizing to a fixed volume, any sequence of minimizers converges to the ball as the mass

goes to infinity. Finally, M. Pegon shows that the threshold on the first moment of the kernels is sharp, in the sense that large balls go from stable to unstable. A direct consequence of the instability of large balls above this threshold is that there exist nontrivial compactly supported kernels for which the problems admit minimizers which are not balls, that is, symmetry breaking occurs.

6.7 Approximation theory

In [31], M. Herda et al. propose an iterative algorithm for the numerical computation of sums of squares of polynomials approximating given data at prescribed interpolation points. The method is based on the definition of a convex functional G arising from the dualization of a quadratic regression over the Cholesky factors of the sum of squares decomposition. In order to justify the construction, the domain of G, the boundary of the domain, and the behavior at infinity are analyzed in details. When the data interpolate a positive univariate polynomial, M. Herda et al. show that in the context of the Lukacs sum of squares representation, G is coercive and strictly convex, which yields a unique critical point and a corresponding decomposition in sum of squares. For multivariate polynomials which admit a decomposition in sum of squares, and up to a small perturbation of size ε, G^ε is always coercive, and so its minimum yields an approximate decomposition in sum of squares. Various unconstrained descent algorithms are proposed to minimize G. Numerical examples are provided, for univariate and bivariate polynomials.

In [18], M. Herda et al. investigate the numerical approximation of bounded functions by polynomials satisfying the same bounds. The contribution makes use of the recent algebraic characterization found in [91, 92], where an interpretation of monovariate polynomials with two bounds is provided in terms of a quaternion algebra and the Euler four-squares formulas. Thanks to this structure, M. Herda et al. generate a new nonlinear projection algorithm onto the set of polynomials with two bounds. The numerical analysis of the method provides theoretical error estimates showing stability and continuity of the projection. Some numerical tests illustrate this novel algorithm for constrained polynomial approximation.

7 Bilateral contracts and grants with industry

7.1 Bilateral contracts with industry

The PhD thesis of S. Bassetto is funded by IFPEn. The contract follows the lines of the bilateral contract between Inria and IFPEn.

7.2 Bilateral grants with industry

CEA (C. Bataillon) and ANDRA (L. Trenty) are involved in the EURAD project on corrosion modeling together with the RAPSODI project-team (C. Cancès, C. Chainais-Hillairet, B. Merlet, and F. Raimondi). More details can be found in Section 8.2.1.

8 Partnerships and cooperations

8.1 International research visitors

8.1.1 Visits of international scientists

M. Breden (École Polytechnique) and A. Zurek (TU Vienna, Austria) spent one week in March 2020 in the team in order to work with C. Chainais-Hillairet on computer-assisted proofs for a corrosion model in the framework of the CNRS NEEDS project POCO (see Section 8.3.3).

8.1.2 Visits to international teams

C. Cancès was invited during one week in Paris in March 2020 to collaborate with V. Ehrlacher and L. Monasse in the framework of the ANR project COMODO (see Section 8.3.1).

8.2 European initiatives

8.2.1 FP7 & H2020 Projects

C. Cancès, C. Chainais-Hillairet, B. Merlet, and F. Raimondi are involved in the H2020 project EURAD (EUropean Joint Programme on RADioactive Waste Management). The aim of their task inside EURAD is to establish an energetic formulation of the Diffusion Poisson Coupled Model leading to new long-time robust numerical methods for the simulation of the corrosion processes in an underground repository. The post-doc position of F. Raimondi is funded by EURAD.

S. Lemaire is a member of the team of D. A. Di Pietro in the ANR MRSEI (Montage de Réseaux Scientifiques Européens ou Internationaux) project NEMESIS (NEw MEthods for numerical SImulationS) funded within the 2020 call. The purpose of this project is to lay the ground for the submission of an ERC Synergy Grant (SyG) within the new Horizon Europe programme, whose goal will be the development of the next generation of numerical simulators for problems governed by PDEs. The SyG project will involve four P.I.s and their teams: P. Antonietti (Politecnico di Milano, Italy), L. Beirão da Veiga (Università di Milano Bicocca, Italy), D. A. Di Pietro (Université de Montpellier, France), and J. Droniou (Monash University, Australia).

8.2.2 Collaborations in European programs, except FP7 and H2020

M. Herda is the French P.I. of a bilateral French-Austrian PHC AMADEUS 2021 program. The two-year project is titled “Design and analysis of structure-preserving numerical schemes for cross-diffusion systems” and has been submitted in collaboration with an Austrian research team at the Institute for Analysis and Scientific Computing, TU Vienna (Austria). The project involves other members of the RAPSODI project-team (C. Cancès, C. Chainais-Hillairet, B. Gaudeul, and T. Rey). The funding (approximately 2000 euros/year) will be used to finance travels of the French members to the Austrian lab to work on the project.

8.3 National initiatives

8.3.1 ANR

C. Chainais-Hillairet and T. Rey are members of the ANR JCJC project MOHYCON. The MOHYCON project is related to the analysis and simulation of multiscale models of semiconductors. As almost all current electronic technology involves the use of semiconductors, there is a strong interest for modeling and simulating the behavior of such devices, which was recently reinforced by the development of organic semiconductors used for example in solar panels or in mobile phones and television screens (among others).

- Title: Multiscale MOdels and HYbrid numerical methods for semiCONductors
- Type: Mathématiques (CE40) - 2017
- ANR reference: ANR-17-CE40-0027
- Duration: January 2018 - March 2022
- Budget: 113 940 euros
- Coordinator: M. Bessemoulin-Chatard (CNRS and Université de Nantes)

C. Cancès is a member of the ANR JCJC project COMODO. The COMODO project focuses on the mathematical and numerical study of cross-diffusion systems in moving domains. The targeted application is the simulation of the production of photovoltaic devices by a vapor deposition process.

- Title: CrOss-diffusion equations in MOving DOmains
- Type: Modèles numériques, simulation, applications (CE46) - 2019
- ANR reference: ANR-19-CE46-0002

- Duration: January 2020 - December 2023
- Budget: 213 810 euros
- Coordinator: V. Ehrlacher (École des Ponts ParisTech and Inria Paris MATHERIALS project-team)

C. Cancès and M. Herda are members of the ANR JCJC project MICMOV. The MICMOV project aims at gathering PDE analysts, probability theorists, and theoretical physicists to work on the derivation of macroscopic properties of physical systems from their microscopic description. The rigorous microscopic description of moving interfaces, the understanding of macroscopic nonlocal effects, and the mathematical apprehension of the underlying atomic mechanisms, are particularly important matters of this project.

- Title: MICroscopic description of MOVing interfaces
- Type: Mathématiques (CE40) - 2019
- ANR reference: ANR-19-CE40-0012
- Duration: February 2020 - January 2024
- Budget: 132 256 euros
- Coordinator: M. Simon (Inria Lille – Nord Europe PARADYSE project-team)

8.3.2 LabEx CEMPI

Through their affiliation to the Laboratoire de mathématiques Paul Painlevé of Université de Lille, RAPSODI team members benefit from the support of the LabEx CEMPI.

- Title: Centre Européen pour les Mathématiques, la Physique et leurs Interactions
- ANR reference: 11-LABX-0007
- Duration: February 2012 - December 2024 (the project has been renewed in 2019)
- Partners: Laboratoire Paul Painlevé (LPP) and Laser Physics department (PhLAM), Université de Lille
- Budget: 6 960 395 euros
- Coordinator: E. Fricain (LPP, Université de Lille)

The “Laboratoire d’Excellence” CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions), a project of the Laboratoire de mathématiques Paul Painlevé (LPP) and the laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), was created in the context of the “Programme d’Investissements d’Avenir” in February 2012.

The association Painlevé-PhLAM creates in Lille a research unit for fundamental and applied research and for training and technological development that covers a wide spectrum of knowledge stretching from pure and applied mathematics to experimental and applied physics.

One of the three focus areas of CEMPI research is the interface between mathematics and physics. This focus area encompasses three themes. The first is concerned with key problems of a mathematical, physical and technological nature coming from the study of complex behavior in cold atoms physics and nonlinear optics, in particular fiber optics. The two other themes deal with fields of mathematics such as algebraic geometry, modular forms, operator algebras, harmonic analysis and quantum groups that have promising interactions with several branches of theoretical physics.

The post-doc position of M. Pegon is funded by the LabEx CEMPI.

8.3.3 CNRS NEEDS

C. Chainais-Hillairet is a member of the CNRS NEEDS (Nucléaire, Énergie, Environnement, Déchets, Société) project POCO (Preuves assistées par Ordinateur pour un modèle de COrrosion) coordinated by M. Breden from École Polytechnique. This project focuses on computer-assisted proofs for a corrosion model (see [48]).

8.4 Regional initiatives

8.4.1 ERC Generator

The MANAKINEQO (MAthematical and Numerical Advances in KINetic EQuatiOns) project (R-ERCGEN-19-007-REY) is a proposal funded (116 545 euros) within the ERC Generator program from I-SITE ULNE. Between February 2020 and May 2022, T. Rey, P.I. of the project, aims at investigating mathematical properties, as well as developing efficient numerical schemes, for multiscale collisional kinetic equations of the Boltzmann type. The 18-month post-doc of R. Bailo is funded using this grant, as well as some planned international events. Following this ERC Generator grant, T. Rey will apply for an ERC Consolidator Grant (CoG).

8.4.2 Actions of Technological Development (ADT)

S. Lemaire is the P.I. of the ADT project ParaSkel++ (funded by the Inria Lille – Nord Europe research center), that started in February 2020. The aim of the project is to develop an optimized C++ platform for the arbitrary-order numerical approximation of PDEs by skeletal methods on general 2/3D meshes, with a particular emphasis on the implementation of HPC facilities. L. Beaude has been hired as a research engineer for this project (more details in Section 5.1).

In the same vein, T. Rey is part of the ADT project SIMPAPH (funded by the Inria Lille – Nord Europe research center) led by the PARADYSE project-team. The aim is to develop robust numerical methods to solve large systems of stochastic differential equations describing (among others) particles in an optic fiber, schools of fish, or microscopic particles. The expected code will attempt to solve these multiscale problems using different approaches, and to be versatile enough to act as an industrial benchmark. A. Roget has been hired as a research engineer for this project.

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

C. Cancès organized the scientific meeting of the GdR MaNu on October 15, held online because of the sanitary crisis. He was also part of the organization committee of the DONUT work-package annual meeting of the EURAD H2020 project, held remotely on May 19-20.

C. Calgaro and I. Lacroix-Violet co-organized with O. Goubet (Université de Lille) the second edition of the Applied Analysis day in Hauts-de-France, that was held remotely on November 26.

E. Creusé was part of the organizing committee of the second "Rencontres Mathématiques Valenciennoises", that were held on March 12 in Valenciennes. This meeting was organized for maths students at Université Polytechnique Hauts-de-France as well as for high-school students of Lycée Wallon in Valenciennes. Several researchers presented some applications of mathematics in industry as well as in academic research.

9.1.2 Scientific events: selection

C. Cancès and C. Chainais-Hillairet were members of the scientific committee of the ninth International Symposium on Finite Volumes for Complex Applications (FVCA IX) originally planned to be held in Bergen (Norway) and which was finally organized remotely on June 15-19.

C. Chainais-Hillairet is a member of the scientific committee of the tenth SMAI congress to be held in May-June 2021 in La Grande-Motte.

9.1.3 Journal

Member of the editorial boards C. Chainais-Hillairet is a member of the editorial board of the North-Western European Journal of Mathematics.

Reviewer - reviewing activities RAPSODI team members are regular reviewers for all the main international journals in PDEs, numerical analysis, and scientific computing.

9.1.4 Invited talks

R. Bailo was invited to give seminars at the University of Warwick and the University of Nottingham (United Kingdom), and at Institut Camille Jordan (Lyon).

C. Calgaro and E. Creusé presented a poster in the ninth International Symposium on Finite Volumes for Complex Applications (FVCA IX), held online on June 15-19.

C. Cancès gave an introductive talk on generalized gradient flows and their applications to complex porous media flows in the framework of the annual Inria-IFPEn meeting.

C. Chainais-Hillairet was an invited speaker in the Workshop 2020 on Partial Differential Equations, held online on September 21-24. She also gave a seminar in Amiens.

F. Chave gave a talk in the FVCA IX conference, held online on June 15-19.

B. Gaudeul participated to the SEME (Semaine d'Études Maths-Entreprises) held in Orléans in January. In exchange for one-week housing and feeding, he contributed to the development of a nonlinear conservative model to reconstruct the water quality in the whole hydrologic system from discrete measures. B. Gaudeul was also a contributed speaker in the FVCA IX conference, held online on June 15-19. He also presented a poster at this conference.

M. Herda presented a poster at the FVCA IX conference, held online on June 15-19. He also gave an online talk in the seminar of C. Mouhot's group in Cambridge University (United Kingdom).

I. Lacroix-Violet gave several seminars in Université Sorbonne Paris Nord, Université de Franche-Comté, and École Polytechnique.

S. Lemaire gave a talk in the ALGORITMY 2020 conference, that was planned to take place in Podbanské (Slovakia) and was finally held remotely on September 10-15.

A. Natale gave an online seminar at the Université Savoie Mont-Blanc.

M. Pegon gave an online seminar at ETH Zürich on September 29.

T. Rey was an invited plenary speaker in the Applied Analysis day in Hauts-de-France, which was held online on November 26. He also gave an online talk on October 15 at the Cambridge Kinetic Coffee, which is a weekly seminar being held usually in the DPMMS of Cambridge. He finally presented a poster at the FVCA IX conference, held online on June 15-19.

9.1.5 Leadership within the scientific community

C. Cancès has headed the CNRS research group GdR MaNu (GdR 2439) on "Mathématiques pour le Nucléaire" until the end of 2020.

C. Cancès is the leader of the task on "Numerical methods for high-performance computing of coupled processes" within the European joint project H2020 EURAD on the management of nuclear waste at the European level (see Section 8.2.1).

9.1.6 Research administration

C. Cancès is a member of the Bureau Scientifique de Centre (BSC) at the Inria Lille – Nord Europe research center, which is a kind of scientific advisory board.

C. Chainais-Hillairet is vice-director of the Laboratoire Paul Painlevé, in charge of human resources for researchers, professors and assistant professors. She is also an elected member of the Conseil de la Faculté des Sciences et Technologies of Université de Lille.

B. Gaudeul is the delegate of the PhD students at the Commission Mixte, and is a member of the Commission Égalité, whose aim is to fight against gender-based discriminations.

M. Herda is the co-organizer of the weekly Numerical Analysis and PDEs (ANEDP) seminar of the Laboratoire Paul Painlevé. He is also an elected member of the Conseil de Laboratoire and of the

Commission Mixte. M. Herda was also appointed substitute member of the Inria Lille – Nord Europe center committee.

I. Lacroix-Violet is a member of the Conseil de la Fédération de Recherche des Hauts-de-France and of the Commission Emploi Recherche (CER) from Inria Lille – Nord Europe research center.

S. Lemaire is a member of the Commission de Développement Technologique (CDT) of the Inria Lille – Nord Europe research center.

B. Merlet is in charge of the Numerical Analysis and PDEs (ANEDP) team of the Laboratoire Paul Painlevé. He is also a member of the Commission Mixte.

T. Rey is a member of the Opération Postes, and the local correspondent of the biomath-oriented research group GdR MathSaV on "Mathématiques, Santé, Sciences de la Vie".

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

RAPSODI team members are strongly involved in teaching at Université de Lille (and UPHF).

Faculty members of the project-team ensure their teaching duties, as well as important administrative tasks in the Mathematics Departments. C. Calgaro is in charge of the Master 1 "Mathematics and Applications", and is a member of the Mathematics Department Council of Université de Lille. B. Merlet is in charge of the Master 2 "Scientific Computing". I. Lacroix-Violet is responsible of the Prod2A's third year at Polytech Lille engineering school. Until the end of 2020, E. Creusé has been the director of the Mathematics Department of INSA/UPHF.

Inria members of the project-team also take part in teaching activities. In 2020, C. Cancès taught a course on "Fundamental notions in Mathematics" (32h) in the framework of the Master 1 "Data Science" of Université de Lille and École Centrale Lille during the months of September and October. F. Chave taught "Numerical Analysis" classes (60h) to second-year students of the Polytech Lille engineering school. S. Lemaire gave lectures (33h) on "Mathematical Tools for Simulation" in the Master 2 "Scientific Computing" at Université de Lille.

9.2.2 Supervision

Research engineer in progress: L. Beaude, on the development of the ParaSkel++ platform, supervised by S. Lemaire, since February 2020, funded by Inria (ADT ParaSkel++).

Post-doc in progress: F. Raimondi, on the "Variational modeling of corrosion", co-advised by C. Cancès, C. Chainais-Hillairet, and B. Merlet, since October 2020, funded by the H2020 EJP EURAD.

Post-doc in progress: M. Pegon, on "Theoretical shape optimization problems", advised by B. Merlet, since September 2020, funded by the LabEx CEMPI.

Post-doc in progress: R. Bailo, on the "Projective Integration of the multiple-species Boltzmann equation", advised by T. Rey, since June 2020, funded by the ERC Generator project MANAKINEQO.

Post-doc: I. Honoré, on the "Large-time behavior of numerical schemes for kinetic equations", advised by M. Herda, from January to August 2020, funded by Inria. The contract ended prematurely as I. Honoré obtained an assistant professor position in Lyon starting from the fall semester.

Post-doc: F. Chave, on "High-order polytopal discretization methods for electromagnetism", advised by S. Lemaire, from December 2018 to July 2020, funded by Inria.

PhD in progress: J. Moatti, on the "Design and analysis of high-order methods for convection-diffusion models, study of the long-time behavior", co-supervised by C. Chainais-Hillairet, M. Herda, and S. Lemaire, since October 2020, funded by Inria (CORDI-S).

PhD in progress: A. Nahas, on "Vortices in Bose–Einstein condensates", co-supervised by G. Dujardin (Inria Lille – Nord Europe PARADYSE project-team) and I. Lacroix-Violet, since September 2019, half funded by the LabEx CEMPI and by the project-team PARADYSE.

PhD in progress: S. Bassetto, on "Towards a more robust and accurate treatment of capillary effects in multiphase flow simulations in porous media", co-supervised by C. Cancès, G. Enchéry (IFPEn), and Q.-H. Tran (IFPEn), since January 2019, funded by IFPEn.

PhD in progress: B. Gaudeul, on the "Numerical approximation of cross-diffusion systems arising in physics and biology", co-supervised by C. Cancès and C. Chainais-Hillairet, since September 2018, funded by Université de Lille (ENS fellowship).

M2 internship: L. Romanowicz (M2 MOS, UPHF), on the “High-order numerical approximation of electromagnetic systems”, co-supervised by F. Chave, S. Lemaire, and Y. Le Menach (L2EP, Université de Lille), from March 16 to August 28, half funded by the L2EP.

M2 internship: J. Moatti (ENS de Lyon), on the “Design and analysis of Hybrid Finite Volume schemes robust in long time for convection-diffusion models”, co-supervised by C. Chainais-Hillairet, M. Herda, and S. Lemaire, from April 1 to July 31.

M1 internship: D. Manouvriez (ESIEE), on “A high-order numerical method for the Benjamin–Ono equation of fluid dynamics”, co-supervised by C. Calgaro and T. Rey, from June 1 to August 31.

M1 internship: G. Helbecque (M1 SC, Université de Lille), on the “Mathematical modeling of the covid-19 epidemics in France”, supervised by T. Rey, from June 1 to July 31.

M1 internship: E. Roubinowitz (M1 SC, Université de Lille), on the “Implementation of numerical methods for the time integration of the nonlinear Schrödinger equation for problems arising in optics”, co-supervised by G. Dujardin (Inria Lille – Nord Europe PARADYSE project-team) and I. Lacroix-Violet, from June 1 to July 31, funded by the PARADYSE project-team.

M1 project (M1 SC, Université de Lille): O. El Outmani, on “The KdV equation: mathematical properties and numerical simulations”, supervised by C. Calgaro.

M1 project (M1 MOS, UPHF): S. Amzin, C. Elbaraka, and A. El Omary, on the “Numerical simulation of the evolution of an antibody in a tumor”, supervised by E. Creusé.

M1 project (M1 SC, Université de Lille): G. Helbecque and Z. Yu, on “Transport equations on networks”, supervised by T. Rey.

9.2.3 Juries

E. Creusé reported on G. Nassreddine’s PhD thesis (Université Sorbonne Paris Nord), titled “Estimations a posteriori pour la simulation des grandes échelles en mécanique des fluides incompressibles” and defended on December 15.

9.3 Popularization

9.3.1 Articles and contents

C. Calgaro and E. Creusé have collaborated twice with an artist (G. Robillard). The first time, this meeting resulted in a script for the voice-over of a film and a graphic work linked to the Navier–Stokes model (see [60]). In the second collaboration (see [61]), the process of creating begins with a didactic phase on the physical significance of dissipative phenomena, and the development of a code for the simulation of fluid flows, where digital matrices are also the objects studied by the artist.

The work of C. Cancès in the framework of the ANR project COMODO (see Section 8.3.1) has inspired an article in the June 2020 issue of the magazine Lille by Inria (page 8).

The obtention of the PHC Amadeus 2021 grant by RAPSODI team members (see Section 8.2.2) has inspired an article in the December 2020 issue of the magazine Lille by Inria (page 10).

9.3.2 Education

B. Gaudeul helped three middle-school interns unravel the arcanes of the Finite Volume discretization of Burger’s equation.

9.3.3 Interventions

C. Calgaro is in charge of the communication of the Laboratoire Paul Painlevé. She also regularly gives or organizes conferences in high-schools in the framework of the “Mathématiques itinérantes”.

C. Calgaro and E. Creusé were invited speakers in the art/science debate “Mettre en scène les mathématiques”, animated by S. Jach and with (as well) E. Liotard, G. Robillard, and V. Vassalo, held on March 12 in Valenciennes. E. Creusé also gave popularization talks on the “Modeling of the impact of antibodies on a tumor” in the Laboratoire de Mathématiques du Lycée Henri Wallon in Valenciennes, on January 23 and February 6.

T. Rey gave a popularization talk on the Twitch channel “Parlons Maths” on April 24.

10 Scientific production

10.1 Major publications

[1] M. Bessemoulin-Chatard and C. Chainais-Hillairet. 'Exponential decay of a finite volume scheme to the thermal equilibrium for drift–diffusion systems'. In: *Journal of Numerical Mathematics* 25.3 (2017), pp. 147–168. DOI: 10.1515/jnma-2016-0007. URL: https://hal.archives-ouvertes.fr/hal-01250709.

[2] C. Calgaro, E. Creusé, T. Goudon and S. Krell. 'Simulations of non homogeneous viscous flows with incompressibility constraints'. In: *Mathematics and Computers in Simulation* 137 (2017), pp. 201–225. URL: https://hal.archives-ouvertes.fr/hal-01246070.

[3] C. Cancès, T. Gallouët and L. Monsaingeon. 'Incompressible immiscible multiphase flows in porous media: a variational approach'. In: *Analysis & PDE* 10.8 (2017), pp. 1845–1876. DOI: 10.2140/apde.2017.10.1845. URL: https://hal.archives-ouvertes.fr/hal-01345438.

[4] C. Cancès and C. Guichard. 'Numerical analysis of a robust free energy diminishing Finite Volume scheme for parabolic equations with gradient structure'. In: *Foundations of Computational Mathematics* 17.6 (2017), pp. 1525–1584. URL: https://hal.archives-ouvertes.fr/hal-01119735.

[5] C. Chainais-Hillairet, B. Merlet and A. Vasseur. 'Positive Lower Bound for the Numerical Solution of a Convection-Diffusion Equation'. In: *FVCA8 2017 - International Conference on Finite Volumes for Complex Applications VIII*. Lille, France: Springer, June 2017, pp. 331–339. DOI: 10.1007/978-3-319-57397-7_26. URL: https://hal.archives-ouvertes.fr/hal-01596076.

[6] D. A. Di Pietro, A. Ern and S. Lemaire. 'An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators'. In: *Computational Methods in Applied Mathematics* 14.4 (June 2014), pp. 461–472. DOI: 10.1515/cmam-2014-0018. URL: https://hal.archives-ouvertes.fr/hal-00978198.

[7] G. Dimarco, R. Loubère, J. Narski and T. Rey. 'An efficient numerical method for solving the Boltzmann equation in multidimensions'. In: *Journal of Computational Physics* 353 (2018), pp. 46–81. DOI: 10.1016/j.jcp.2017.10.010. URL: https://hal.archives-ouvertes.fr/hal-01357112.

[8] F. Filbet and M. Herda. 'A finite volume scheme for boundary-driven convection-diffusion equations with relative entropy structure'. In: *Numerische Mathematik* 137.3 (2017), pp. 535–577. URL: https://hal.archives-ouvertes.fr/hal-01326029.

[9] I. Lacroix-Violet and A. Vasseur. 'Global weak solutions to the compressible quantum Navier–Stokes equation and its semi-classical limit'. In: *Journal de Mathématiques Pures et Appliquées* 114 (2018), pp. 191–210. URL: https://hal.archives-ouvertes.fr/hal-01347943.

[10] B. Merlet. 'A highly anisotropic nonlinear elasticity model for vesicles I. Eulerian formulation, rigidity estimates and vanishing energy limit'. In: *Arch. Ration. Mech. Anal.* 217.2 (2015), pp. 651–680. DOI: 10.1007/s00205-014-0839-5. URL: https://hal.archives-ouvertes.fr/hal-00848547.

10.2 Publications of the year

International journals

[11] F. Alouges, A. de Bouard, B. Merlet and L. Nicolas. 'Stochastic homogenization of the Landau-Lifshitz-Gilbert equation'. In: *Stochastics and Partial Differential Equations: Analysis and Computations* (2nd Jan. 2021). DOI: 10.1007/s40072-020-00185-4. URL: https://hal.archives-ouvertes.fr/hal-02020241.

[12] N. Ayi, M. Herda, H. Hivert and I. Tristani. 'A note on hypocoercivity for kinetic equations with heavy-tailed equilibrium'. In: *Comptes Rendus Mathématique* 358.3 (10th July 2020), pp. 333–340. DOI: 10.5802/crmath.46. URL: https://hal.archives-ouvertes.fr/hal-02389146.

[13] R. Bailo, J. A. Carrillo, H. Murakawa and M. Schmidtchen. 'Convergence of a fully discrete and energy-dissipating finite-volume scheme for aggregation-diffusion equations'. In: *Mathematical Models and Methods in Applied Sciences* 30.13 (2020), pp. 2487–2522. DOI: 10.1142/S0218202520500487. URL: https://hal.archives-ouvertes.fr/hal-03125839.

[14] C. Besse, S. Descombes, G. Dujardin and I. Lacroix-Violet. 'Energy preserving methods for nonlinear Schrödinger equations'. In: *IMA Journal of Numerical Analysis* 41.1 (Jan. 2021), pp. 618–653. DOI: 10.1093/imanum/drz067. URL: https://hal.archives-ouvertes.fr/hal-01951527.

[15] M. Bessemoulin-Chatard, M. Herda and T. Rey. 'Hypocoercivity and diffusion limit of a finite volume scheme for linear kinetic equations'. In: *Mathematics of Computation* 89 (Jan. 2020), pp. 1093–1133. DOI: 10.1090/mcom/3490. URL: https://hal.archives-ouvertes.fr/hal-01957832.

[16] S. Billiard, M. Derex, L. Maisonneuve and T. Rey. 'Convergence of knowledge in a stochastic cultural evolution model with population structure, social learning and credibility biases'. In: *Mathematical Models and Methods in Applied Sciences* 30.14 (7th Dec. 2020), pp. 2691–2723. DOI: 10.1142/S0218202520500529. URL: https://hal.archives-ouvertes.fr/hal-02357188.

[17] C. Calgaro, C. Colin and E. Creusé. 'A combined finite volume - finite element scheme for a low-Mach system involving a Joule term'. In: *AIMS Mathematics* 5.1 (2020), pp. 311–331. DOI: 10.3934/math.2020021. URL: https://hal.archives-ouvertes.fr/hal-02398893.

[18] M. Campos Pinto, F. Charles, B. Després and M. Herda. 'A projection algorithm on the set of polynomials with two bounds'. In: *Numerical Algorithms* 85 (4th Feb. 2020), pp. 1475–1498. DOI: 10.1007/s11075-019-00872-x. URL: https://hal.archives-ouvertes.fr/hal-02128851.

[19] C. Cancès, C. Chainais-Hillairet, J. Fuhrmann and B. Gaudeul. 'A numerical analysis focused comparison of several Finite Volume schemes for an Unipolar Degenerated Drift-Diffusion Model'. In: *IMA Journal of Numerical Analysis* 41.1 (2021), pp. 271–314. DOI: 10.1093/imanum/draa002. URL: https://hal.archives-ouvertes.fr/hal-02194604.

[20] C. Cancès, C. Chainais-Hillairet, M. Herda and S. Krell. 'Large time behavior of nonlinear finite volume schemes for convection-diffusion equations'. In: *SIAM Journal on Numerical Analysis* 58.5 (16th Sept. 2020), pp. 2544–2571. DOI: 10.1137/19M1299311. URL: https://hal.archives-ouvertes.fr/hal-02360155.

[21] C. Cancès, T. Gallouët and G. Todeschi. 'A variational finite volume scheme for Wasserstein gradient flows'. In: *Numerische Mathematik* 146.3 (2020), pp 437 –480. DOI: 10.1007/s00211-020-01153-9. URL: https://hal.archives-ouvertes.fr/hal-02189050.

[22] C. Cancès and B. Gaudeul. 'A convergent entropy diminishing finite volume scheme for a cross-diffusion system'. In: *SIAM Journal on Numerical Analysis* 58.5 (2020), pp. 2784–2710. DOI: 10.1137/20M1316093. URL: https://hal.archives-ouvertes.fr/hal-02465431.

[23] C. Cancès, D. Granjeon, Q.-H. Tran, S. Wolf and N. Peton. 'Numerical scheme for a water flow-driven forward stratigraphic model'. In: *Computational Geosciences* 24 (2020), pp. 37–60. DOI: 10.1007/s10596-019-09893-w. URL: https://hal.archives-ouvertes.fr/hal-01870347.

[24] C. Cancès and D. Maltese. 'A gravity current model with capillary trapping for oil migration in multilayer geological basins'. In: *SIAM Journal on Applied Mathematics* 81.2 (2021), pp. 454–484. DOI: 10.1137/19M1284233. URL: https://hal.archives-ouvertes.fr/hal-02272965.

[25] C. Cancès and F. Nabet. 'Finite Volume approximation of a two-phase two fluxes degenerate Cahn-Hilliard model'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* (2021). DOI: 10.1051/m2an/2021002. URL: https://hal.archives-ouvertes.fr/hal-02561981.

[26] C. Cancès, F. Nabet and M. Vohralík. 'Convergence and a posteriori error analysis for energy-stable finite element approximations of degenerate parabolic equations'. In: *Mathematics of Computation* 90 (2021), pp. 517–563. DOI: 10.1090/mcom/3577. URL: https://hal.archives-ouvertes.fr/hal-01894884.

[27] C. Chainais-Hillairet and M. Herda. 'Large-time behaviour of a family of finite volume schemes for boundary-driven convection-diffusion equations'. In: *IMA Journal of Numerical Analysis* 40.4 (1st Oct. 2020), pp. 2473–2505. DOI: 10.1093/imanum/drz037. URL: https://hal.archives-ouvertes.fr/hal-01885015.

[28] A. Chambolle, L. A. D. Ferrari and B. Merlet. 'Strong approximation in h-mass of rectifiable currents under homological constraint'. In: *Advances in Calculus of Variation* (2021). DOI: 10.1515/acv-2018-0079. URL: https://hal.archives-ouvertes.fr/hal-01813234.

[29] E. Creusé, S. Nicaise and R. V. Sabariego. 'Existence results for the $\mathbf{A}-\varphi-\mathbf{B}$ magnetodynamic formulation of the Maxwell system with skin and proximity effects'. In: *Applicable Analysis* (2021). DOI: 10.1080/00036811.2020.1836351. URL: https://hal.archives-ouvertes.fr/hal-03122785.

[30] P. Degond, M. Herda and S. Mirrahimi. 'A Fokker-Planck approach to the study of robustness in gene expression'. In: *Mathematical Biosciences and Engineering* 17.6 (24th Sept. 2020), pp. 6459–6486. DOI: 10.3934/mbe.2020338. URL: https://hal.archives-ouvertes.fr/hal-02882349.

[31] B. Després and M. Herda. 'Computation of sum of squares polynomials from data points'. In: *SIAM Journal on Numerical Analysis* 58.3 (2020), pp. 1719–1743. DOI: 10.1137/19M1273955. URL: https://hal.archives-ouvertes.fr/hal-01946539.

[32] M. Goldman and B. Merlet. 'Non-convex functionals penalizing simultaneous oscillations along independent directions: rigidity estimates'. In: *Annali della Scuola Normale Superiore di Pisa, Classe di Scienze* (2021). URL: https://hal.archives-ouvertes.fr/hal-02132896.

[33] M. Goldman, B. Merlet and V. Millot. 'A Ginzburg-Landau model with topologically induced free discontinuities'. In: *Annales de l'Institut Fourier* (2021). URL: https://hal.archives-ouvertes.fr/hal-01643795.

[34] S. Lemaire. 'Bridging the Hybrid High-Order and Virtual Element methods'. In: *IMA Journal of Numerical Analysis* 41.1 (2021), pp. 549–593. DOI: 10.1093/imanum/drz056. URL: https://hal.archives-ouvertes.fr/hal-01902962.

International peer-reviewed conferences

[35] S. Bassetto, C. Cancès, G. Enchéry and Q. H. Tran. 'Robust Newton solver based on variable switch for a finite volume discretization of Richards equation'. In: Finite Volumes for Complex Applications IX. Bergen, Norway, 2020. URL: https://hal.archives-ouvertes.fr/hal-02464945.

[36] M. Bessemoulin-Chatard, C. Chainais-Hillairet and H. Mathis. 'Numerical schemes for semiconductors energy- transport models'. In: Finite Volumes for Complex Applications IX. Vol. vol. 323 of Springer Proceedings in Mathematics and Statistics. Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples (R. Klöfkorn, E. Keilegavlen, F. A. Radu, and J. Fuhrmann, eds.), Bergen, Norway: Springer, Cham, 15th June 2020, pp. 75–90. URL: https://hal.archives-ouvertes.fr/hal-02563093.

[37] C. Calgaro and E. Creusé. 'A finite volume method for a convection- diffusion equation involving a Joule term'. In: International Conference on Finite Volumes for Complex Applications IX. Vol. 323. Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples. Bergen, Norway, 2020, pp. 405–413. DOI: 10.1007/978-3-030-43651-3_37. URL: https://hal.inria.fr/hal-02432936.

[38] C. Cancès, C. Chainais-Hillairet, J. Fuhrmann and B. Gaudeul. 'On four numerical schemes for a unipolar degenerate drift-diffusion model'. In: Finite Volumes for Complex Applications IX. Bergen, Norway, 2020. URL: https://hal.archives-ouvertes.fr/hal-02461524.

[39] C. Cancès and B. Gaudeul. 'Entropy diminishing finite volume approximation of a cross-diffusion system'. In: FVCA9 - International Conference on Finite Volumes for Complex Applications IX. Bergen, Norway, 2020. URL: https://hal.archives-ouvertes.fr/hal-02418908.

[40] C. Cancès and F. Nabet. 'Energy stable discretization for two-phase porous media flows'. In: Finite Volumes for Complex Applications IX. Bergen, Norway, 15th June 2020. URL: https://hal.archives-ouvertes.fr/hal-02442233.

[41] C. Chainais-Hillairet and M. Herda. 'L^∞ bounds for numerical solutions of noncoercive convection-diffusion equations'. In: Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples. Vol. 323. Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples. FVCA 2020. Bergen, Norway, 15th June 2020. DOI: 10.1007/978-3-030-43651-3_12. URL: https://hal.archives-ouvertes.fr/hal-02404546.

[42] C. Chainais-Hillairet and S. Krell. 'Exponential decay to equilibrium of nonlinear DDFV schemes for convection-diffusion equations'. In: FVCA 2020 - 9th Conference on Finite Volumes for Complex Applications. Bergen, Norway, 15th June 2020. URL: https://hal.archives-ouvertes.fr/hal-02408212.

[43] F. Chave, D. A. Di Pietro and S. Lemaire. 'A three-dimensional Hybrid High-Order method for magnetostatics'. In: Finite Volumes for Complex Applications IX. Vol. 323. Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples. Bergen, Norway: Springer, Cham, 2020, pp. 255–263. DOI: 10.1007/978-3-030-43651-3_22. URL: https://hal.archives-ouvertes.fr/hal-02407175.

[44] A. El Keurti and T. Rey. 'Finite Volume Method for a System of Continuity Equations Driven by Nonlocal Interactions'. In: International Conference on Finite Volumes for Complex Applications. FVCA 2020: Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples. Bergen, Norway, 10th June 2020. DOI: 10.1007/978-3-030-43651-3_20. URL: https://hal.archives-ouvertes.fr/hal-02408246.

Scientific book chapters

[45] C. Cancès, J. Droniou, C. Guichard, G. Manzini, M. Bastidas Olivares and I. S. Pop. 'Error estimates for the gradient discretisation of degenerate parabolic equation of porous medium type'. In: *Polyhedral methods in geosciences*. SEMA-SIMAI. Springer, 2021. URL: https://hal.archives-ouvertes.fr/hal-02540067.

Reports & preprints

[46] E. Ahusborde, B. Amaziane, A. Baksay, G. Bator, D. Becker, A. Bednar, M. Beres, R. Blaheta, Z. Böhti, G. Bracke et al. *State Of the Art Report in the fields of numerical analysis and scientific computing. Final version as of 16/02/2020 deliverable D4.1 of the HORIZON 2020 project EURAD.: European Joint Programme on Radioactive Waste Management*. EC Grant agreement no: 847593, 2020. URL: https://hal.archives-ouvertes.fr/hal-03165686.

[47] M. Bessemoulin-Chatard, C. Chainais-Hillairet and H. Mathis. *Analysis of numerical schemes for semiconductors energy-transport models*. 16th Sept. 2020. URL: https://hal.archives-ouvertes.fr/hal-02940224.

[48] M. Breden, C. Chainais-Hillairet and A. Zurek. *Existence of traveling wave solutions for the Diffusion Poisson Coupled Model: a computer-assisted proof*. 18th Dec. 2020. URL: https://hal.archives-ouvertes.fr/hal-03082893.

[49] D. Bresch, M. Gisclon, I. Lacroix-Violet and A. F. Vasseur. *On the Exponential decay for Compressible Navier-Stokes-Korteweg equations with a Drag Term*. 10th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02542115.

[50] C. Cancès, V. Ehrlacher and L. Monasse. *Finite Volumes for the Stefan-Maxwell Cross-Diffusion System*. 20th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02902672.

[51] C. Cancès and D. Matthes. *Construction of a two-phase flow with singular energy by gradient flow methods*. 2020. URL: https://hal.archives-ouvertes.fr/hal-02510535.

[52] C. Cancès and A. Zurek. *A convergent finite volume scheme for dissipation driven models with volume filling constraint*. 2021. URL: https://hal.archives-ouvertes.fr/hal-03166069.

[53] J. Carrillo, J. Hu, Z. Ma and T. Rey. *Recent development in kinetic theory of granular materials: analysis and numerical methods*. 30th Jan. 2020. URL: https://hal.archives-ouvertes.fr/hal-02460375.

[54] F. Chave, D. A. Di Pietro and S. Lemaire. *A discrete Weber inequality on three-dimensional hybrid spaces with application to the HHO approximation of magnetostatics*. 7th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02892526.

[55] G. Dujardin and I. Lacroix-Violet. *High order linearly implicit methods for evolution equations: How to solve an ODE by inverting only linear systems*. 22nd Oct. 2020. URL: https://hal.inria.fr/hal-02361814.

[56] B. Merlet and M. Pegon. *The isoperimetric problem for the perimeter minus a fraction of a nonlocal approximate perimeter in 2D*. 25th Mar. 2021. URL: https://hal.archives-ouvertes.fr/hal-03181775.

[57] A. Natale and G. Todeschi. *Computation of Optimal Transport with Finite Volumes*. 2020. URL: https://hal.archives-ouvertes.fr/hal-03032446.

[58] L. Pareschi and T. Rey. *On the stability of equilibrium preserving spectral methods for the homogeneous Boltzmann equation*. 11th Nov. 2020. URL: https://hal.archives-ouvertes.fr/hal-03000138.

[59] M. Pegon. *Large mass minimizers for isoperimetric problems with integrable nonlocal potentials*. 3rd Nov. 2020. URL: https://hal.archives-ouvertes.fr/hal-02496313.

[60] G. Robillard, C. Calgaro and E. Creusé. *En recherchant la vague*. Université de Lille (2018-....), 2020, 2020:01. URL: https://hal.archives-ouvertes.fr/hal-03133378.

[61] G. Robillard, C. Calgaro and E. Creusé. *The Wave in the Matrix*. Université de Lille (2018-....), 2020, 2020:02. URL: https://hal.archives-ouvertes.fr/hal-03133380.

10.3 Other

Softwares

[62] [SW] A. Mouton, C. Calgaro and E. Creusé, *NS2DDV - Navier-Stokes 2D à Densité Variable*, 10th Apr. 2020. HAL: ⟨hal-02137040⟩, URL: https://hal.archives-ouvertes.fr/hal-02137040, SWHID: ⟨swh:1:dir:ea24497c97c446b847eb1e6b144fc0528b22798f;origin=https://hal.archives-ouvertes.fr/hal-02137040;visit=swh:1:snp:6d9b0a7121ef7aee4569095d3304fd3c77f27314;anchor=swh:1:rev:04a7cf3445bc390bc8dfaf93341a1f8f2008072c;path=/⟩.

10.4 Cited publications

[63] R. Abgrall. 'A review of residual distribution schemes for hyperbolic and parabolic problems: the July 2010 state of the art'. In: *Commun. Comput. Phys.* 11.4 (2012), pp. 1043–1080. DOI: 10.4208/cicp.270710.130711s.

[64] R. Abgrall, G. Baurin, A. Krust, D. de Santis and M. Ricchiuto. 'Numerical approximation of parabolic problems by residual distribution schemes'. In: *Internat. J. Numer. Methods Fluids* 71.9 (2013), pp. 1191–1206. DOI: 10.1002/fld.3710.

[65] R. Abgrall, A. Larat and M. Ricchiuto. 'Construction of very high order residual distribution schemes for steady inviscid flow problems on hybrid unstructured meshes'. In: *J. Comput. Phys.* 230.11 (2011), pp. 4103–4136. DOI: 10.1016/j.jcp.2010.07.035.

[66] R. Abgrall, A. Larat, M. Ricchiuto and C. Tavé. 'A simple construction of very high order non-oscillatory compact schemes on unstructured meshes'. In: *Comput. & Fluids* 38.7 (2009), pp. 1314–1323. DOI: 10.1016/j.compfluid.2008.01.031.

[67] T. Aiki and A. Muntean. 'A free-boundary problem for concrete carbonation: front nucleation and rigorous justification of the $\sqrt{t}$-law of propagation'. In: *Interfaces Free Bound.* 15.2 (2013), pp. 167–180. DOI: 10.4171/IFB/299.

[68] B. Amaziane, A. Bergam, M. El Ossmani and Z. Mghazli. 'A posteriori estimators for vertex centred finite volume discretization of a convection-diffusion-reaction equation arising in flow in porous media'. In: *Internat. J. Numer. Methods Fluids* 59.3 (2009), pp. 259–284. DOI: 10.1002/fld.1456. URL: http://dx.doi.org/10.1002/fld.1456.

[69] I. Babuška and W. C. Rheinboldt. 'Error estimates for adaptive finite element computations'. In: *SIAM J. Numer. Anal.* 15.4 (1978), pp. 736–754.

[70] R. Bailo, J. A. Carrillo and J. Hu. 'Fully Discrete Positivity-Preserving and Energy-Dissipating Schemes for Aggregation-Diffusion Equations with a Gradient Flow Structure'. en. In: *Commun. Math. Sci.* 18.5 (2020), pp. 1259–1303. DOI: 10.4310/CMS.2020.v18.n5.a5.

[71] C. Bataillon, F. Bouchon, C. Chainais-Hillairet, C. Desgranges, E. Hoarau, F. Martin, S. Perrin, M. Tupin and J. Talandier. 'Corrosion modelling of iron based alloy in nuclear waste repository'. In: *Electrochim. Acta* 55.15 (2010), pp. 4451–4467.

[72] J. Bear. *Dynamic of Fluids in Porous Media*. New York: American Elsevier, 1972.

[73] J. Bear and Y. Bachmat. *Introduction to modeling of transport phenomena in porous media*. Vol. 4. Springer, 1990.

[74] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini and A. Russo. 'Basic principles of virtual element methods'. In: *Math. Models Methods Appl. Sci. (M3AS)* 23.1 (2013), pp. 199–214.

[75] S. Berrone, V. Garbero and M. Marro. 'Numerical simulation of low-Reynolds number flows past rectangular cylinders based on adaptive finite element and finite volume methods'. In: *Comput. & Fluids* 40 (2011), pp. 92–112. DOI: 10.1016/j.compfluid.2010.08.014. URL: http://dx.doi.org/10.1016/j.compfluid.2010.08.014.

[76] C. Besse. 'Analyse numérique des systèmes de Davey–Stewartson'. PhD thesis. Université Bordeaux 1, 1998.

[77] M. Bessemoulin-Chatard, C. Chainais-Hillairet and M.-H. Vignal. 'Study of a fully implicit scheme for the drift-diffusion system. Asymptotic behavior in the quasi-neutral limit'. Anglais. In: *SIAM, J. Numer. Anal.* 52.4 (2014). URL: https://epubs.siam.org/doi/abs/10.1137/130913432.

[78] D. Bresch, A. Vasseur and C. Yu. 'Global Existence of Entropy-Weak Solutions to the Compressible Navier-Stokes Equations with Non-Linear Density Dependent Viscosities'. working paper or preprint. 2019. URL: https://arxiv.org/abs/1905.02701.

[79] C. Calgaro, E. Creusé and T. Goudon. 'An hybrid finite volume-finite element method for variable density incompressible flows'. In: *J. Comput. Phys.* 227.9 (2008), pp. 4671–4696.

[80] C. Calgaro, E. Creusé and T. Goudon. 'Modeling and simulation of mixture flows: application to powder-snow avalanches'. In: *Comput. & Fluids* 107 (2015), pp. 100–122. URL: http://dx.doi.org/10.1016/j.compfluid.2014.10.008.

[81] C. Cancès, D. Matthes and F. Nabet. 'A two-phase two-fluxes degenerate Cahn–Hilliard model as constrained Wasserstein gradient flow'. In: *Arch. Ration. Mech. Anal.* 233.2 (2019), pp. 837–866.

[82] C. Cancès, I. S. Pop and M. Vohralík. 'An a posteriori error estimate for vertex-centered finite volume discretizations of immiscible incompressible two-phase flow'. In: *Math. Comp.* 83.285 (2014), pp. 153–188. DOI: 10.1090/S0025-5718-2013-02723-8. URL: http://dx.doi.org/10.1090/S0025-5718-2013-02723-8.

[83] C. Cancès and C. Guichard. 'Convergence of a nonlinear entropy diminishing Control Volume Finite Element scheme for solving anisotropic degenerate parabolic equations'. In: *Mathematics of Computation* 85.298 (2016), pp. 549–580. URL: https://hal.archives-ouvertes.fr/hal-00955091.

[84] J. A. Carrillo, A. Jüngel, P. A. Markowich, G. Toscani and A. Unterreiter. 'Entropy dissipation methods for degenerate parabolic problems and generalized Sobolev inequalities'. In: *Monatsh. Math.* 133.1 (2001), pp. 1–82. DOI: 10.1007/s006050170032. URL: http://dx.doi.org/10.1007/s006050170032.

[85] C. Chainais-Hillairet. 'Entropy method and asymptotic behaviours of finite volume schemes'. In: *Finite volumes for complex applications. VII. Methods and theoretical aspects*. Vol. 77. Springer Proc. Math. Stat. Springer, Cham, 2014, pp. 17–35.

[86] C. Chainais-Hillairet, A. Jüngel and S. Schuchnigg. 'Entropy-dissipative discretization of nonlinear diffusion equations and discrete Beckner inequalities'. In: *Modelisation Mathématique et Analyse Numérique* 50.1 (2016), pp. 135–162. URL: https://hal.archives-ouvertes.fr/hal-00924282.

[87] A. Chambolle, L. A. D. Ferrari and B. Merlet. 'Variational approximation of size-mass energies for k-dimensional currents'. In: *ESAIM: Control, Optimisation and Calculus of Variations* 25 (2019).43 (Sept. 2019), p. 39. DOI: 10.1051/cocv/2018027. URL: https://hal.archives-ouvertes.fr/hal-01622540.

[88] E. Creusé, S. Nicaise, Z. Tang, Y. Le Menach, N. Nemitz and F. Piriou. 'Residual-based *a posteriori* estimators for the $\mathbf{A}-\varphi$ magnetodynamic harmonic formulation of the Maxwell system'. In: *Math. Models Methods Appl. Sci.* 22.5 (2012), pp. 1150028–30. DOI: 10.1142/S021820251150028X. URL: http://dx.doi.org/10.1142/S021820251150028X.

[89] E. Creusé, S. Nicaise, Z. Tang, Y. Le Menach, N. Nemitz and F. Piriou. 'Residual-based a posteriori estimators for the $\mathbf{T}/\Omega$ magnetodynamic harmonic formulation of the Maxwell system'. In: *Int. J. Numer. Anal. Model.* 10.2 (2013), pp. 411–429.

[90] E. Creusé, S. Nicaise and E. Verhille. 'Robust equilibrated a posteriori error estimators for the Reissner-Mindlin system'. In: *Calcolo* 48.4 (2011), pp. 307–335. DOI: 10.1007/s10092-011-0042-0. URL: http://dx.doi.org/10.1007/s10092-011-0042-0.

[91] B. Després. 'Polynomials with bounds and numerical approximation'. In: *Numerical Algorithms* 76.3 (2017), pp. 829–859. DOI: 10.1007/s11075-017-0286-0. URL: https://doi.org/10.1007/s11075-017-0286-0.

[92] B. Després and M. Herda. 'Correction to: Polynomials with bounds and numerical approximation'. In: *Numerical Algorithms* 77.1 (2018), pp. 309–311. DOI: 10.1007/s11075-017-0441-7. URL: https://doi.org/10.1007/s11075-017-0441-7.

[93] D. A. Di Pietro and M. Vohralík. 'A Review of Recent Advances in Discretization Methods, a Posteriori Error Analysis, and Adaptive Algorithms for Numerical Modeling in Geosciences'. In: *Oil & Gas Science and Technology-Rev. IFP* (June 2014). (online first), pp. 1–29.

[94] D. A. Di Pietro, A. Ern and S. Lemaire. 'An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators'. In: *Comput. Methods Appl. Math.* 14.4 (2014), pp. 461–472. DOI: 10.1515/cmam-2014-0018. URL: https://doi.org/10.1515/cmam-2014-0018.

[95] J. Dolbeault, C. Mouhot and C. Schmeiser. 'Hypocoercivity for linear kinetic equations conserving mass'. In: *Trans. Amer. Math. Soc.* 367.6 (2015), pp. 3807–3828. DOI: 10.1090/S0002-9947-2015-06012-7. URL: https://doi.org/10.1090/S0002-9947-2015-06012-7.

[96] V. Dolejší, A. Ern and M. Vohralík. 'A framework for robust a posteriori error control in unsteady nonlinear advection-diffusion problems'. In: *SIAM J. Numer. Anal.* 51.2 (2013), pp. 773–793. DOI: 10.1137/110859282. URL: http://dx.doi.org/10.1137/110859282.

[97] J. Droniou. 'Finite volume schemes for diffusion equations: introduction to and review of modern methods'. In: *Math. Models Methods Appl. Sci.* 24.8 (2014), pp. 1575–1620.

[98] W. E and P. Palffy-Muhoray. 'Phase separation in incompressible systems'. In: *Phys. Rev. E* 55 (4 Apr. 1997), R3844–R3846. DOI: 10.1103/PhysRevE.55.R3844. URL: https://link.aps.org/doi/10.1103/PhysRevE.55.R3844.

[99] [SW] V. Ehrlacher, C. Cancès and L. Monasse, *Finite volume scheme for the Stefan–Maxwell model* version 1.0, July 2020. DOI: 10.5281/zenodo.3934286, URL: https://doi.org/10.5281/zenodo.3934286.

[100] E. Emmrich. 'Two-step BDF time discretisation of nonlinear evolution problems governed by monotone operators with strongly continuous perturbations'. In: *Comput. Methods Appl. Math.* 9.1 (2009), pp. 37–62.

[101] J. de Frutos, B. García-Archilla and J. Novo. 'A posteriori error estimations for mixed finite-element approximations to the Navier-Stokes equations'. In: *J. Comput. Appl. Math.* 236.6 (2011), pp. 1103–1122. DOI: 10.1016/j.cam.2011.07.033. URL: http://dx.doi.org/10.1016/j.cam.2011.07.033.

[102] L. Greengard and J.-Y. Lee. 'Accelerating the nonuniform fast Fourier transform'. In: *SIAM Rev.* 46.3 (2004), pp. 443–454. DOI: 10.1137/S003614450343200X. URL: http://dx.doi.org/10.1137/S003614450343200X.

[103] M. E. Hubbard and M. Ricchiuto. 'Discontinuous upwind residual distribution: a route to unconditional positivity and high order accuracy'. In: *Comput. & Fluids* 46 (2011), pp. 263–269. DOI: 10.1016/j.compfluid.2010.12.023. URL: http://dx.doi.org/10.1016/j.compfluid.2010.12.023.

[104] S. Jin. 'Efficient asymptotic-preserving (AP) schemes for some multiscale kinetic equations'. In: *SIAM, J. Sci. Comput.* 21 (1999), pp. 441–454.

[105] A. Majda and J. Sethian. 'The derivation and numerical solution of the equations for zero Mach number combustion'. In: *Combustion Science and Technology* 42 (1985), pp. 185–205.

[106] F. Otto. 'The geometry of dissipative evolution equations: the porous medium equation'. In: *Comm. Partial Differential Equations* 26.1-2 (2001), pp. 101–174.

[107] M. Ricchiuto and R. Abgrall. 'Explicit Runge-Kutta residual distribution schemes for time dependent problems: second order case'. In: *J. Comput. Phys.* 229.16 (2010), pp. 5653–5691. DOI: 10.1016/j.jcp.2010.04.002. URL: http://dx.doi.org/10.1016/j.jcp.2010.04.002.

[108] D. Ruppel and E. Sackmann. 'On defects in different phases of two-dimensional lipid bilayers'. In: *J. Phys. France* 44.9 (1983), pp. 1025–1034. DOI: 10.1051/jphys:019830044090102500. URL: https://jphys.journaldephysique.org/articles/jphys/abs/1983/09/jphys_1983__44_9_1025_0/jphys_1983__44_9_1025_0.html.

[109] M. Vohralík. 'Residual flux-based a posteriori error estimates for finite volume and related locally conservative methods'. In: *Numer. Math.* 111.1 (2008), pp. 121–158. DOI: 10.1007/s00211-008-0168-4. URL: http://dx.doi.org/10.1007/s00211-008-0168-4.